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14. ABSTRACT
This final report summarizes the results obtained in the project "Controllable, Hubbard-like Correlated Electron Physics in Oxide Quantum Structures'. Results are reported from experiments and theory of oxide interfaces and correlations effects that occur at high-electron densities. SrTiO3/GdTiO3 interfaces served as the platform materials system. Correlated phenomena that appeared in SrTiO3 quantum wells bound by two SrTiO3/GdTiO3 interfaces and magnetism in this system are reported.

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Report Title

Final Report: Controllable, Hubbard-like Correlated Electron Physics in Oxide Quantum Structures

ABSTRACT

This final report summarizes the results obtained in the project "Controllable, Hubbard-like Correlated Electron Physics in Oxide Quantum Structures'. Results are reported from experiments and theory of oxide interfaces and correlations effects that occur at high-electron densities. SrTiO3/GdTiO3 interfaces served as the platform materials system. Correlated phenomena that appeared in SrTiO3 quantum wells bound by two SrTiO3/GdTiO3 interfaces and magnetism in this system are reported.

Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

Received		Paper
04/27/2013	5.00	Ru Chen, SungBin Lee, Leon Balents. Dimer Mott insulator in an oxide heterostructure, Physical Review B, (04 2013): 161119. doi:
05/13/2013	6.00	Gang Chen, Leon Balents. Ferromagnetism in Itinerant Two-Dimensional t2g Systems, Phys. Rev. Lett., (05 2013): 206401. doi:
07/08/2013	7.00	Jack Y. Zhang, Jinwoo Hwang, Santosh Raghavan, Susanne Stemmer. Symmetry Lowering in Extreme-Electron-Density Perovskite Quantum Wells, Physical Review Letters, (06 2013): 256401. doi: 10.1103/PhysRevLett.110.256401
08/12/2014	9.00	Clayton A. Jackson, Susanne Stemmer. Interface-induced magnetism in perovskite quantum wells, Physical Review B, (11 2013): 180403. doi: 10.1103/PhysRevB.88.180403
11/01/2014	10.00	Daniel G. Ouellette, Pouya Moetakef, Tyler A. Cain, Jack Y. Zhang, Susanne Stemmer, David Emin, S. James Allen. High-density Two-Dimensional SmallPolaron Gas in a Delta-Doped Mott Insulator, Scientific Reports, (11 2013): 3284. doi:
11/21/2012	2.00	Pouya Moetakef, Clayton Jackson, Jinwoo Hwang, Leon Balents, S. James Allen, Susanne Stemmer. Toward an artificial Mott insulator: Correlations in confined high-density electron liquids in SrTiO_{3}, Physical Review B, (11 2012): 201102. doi: 10.1103/PhysRevB.86.201102
11/22/2013	8.00	Pouya Moetakef, Tyler A. Cain, Jack Y. Zhang, Susanne Stemmer, Daniel G. Ouellette, David Emin, S. James Allen. High-density Two-Dimensional Small Polaron Gas in a Delta-Doped Mott Insulator, Scientific Reports, (11 2013): 3284. doi: 10.1038/srep03284

TOTAL: 7

Number of Papers published in peer-reviewed journals:

(b) Papers published in non-peer-reviewed journals (N/A for none)

Received Paper

TOTAL:

Number of Papers published in non peer-reviewed journals:

(c) Presentations

Number of Presentations: 0.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

TOTAL:

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

TOTAL:

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts):

(d) Manuscripts

Received		Paper
01/23/2013	3.00	Ru Chen, SungBin Lee, Leon Balents. Dimer Mott Insulator in an Oxide Heterostructure, SUBMITTED (01 2013)
04/23/2013	4.00	Leon Balents, Gang Chen. Ferromagnetism in itinerant two-dimensional t2g systems, Submitted to phys. Rev. Lett. (04 2013)
10/21/2012	1.00	Pouya Moetakef, Clayton A. Jackson, Jinwoo Hwang, Leon Balents, S. James Allen, Susanne Stemmer. Towards an artificial Mott insulator: Correlations in confined, high-density electron liquids in SrTiO3, Submitted to physical review B (10 2012)

TOTAL: **3**

Number of Manuscripts:

Books

Received Book

TOTAL:

Received Book Chapter

TOTAL:

Patents Submitted

Patents Awarded

Awards

Susanne Stemmer: Election to Fellow of the Materials Research Society
Leon Balents: Election to Fellow of the American Physical Society

Graduate Students

NAME	PERCENT_SUPPORTED	Discipline
Ru Chen	0.65	
William Flaherty	0.09	
Daniel Ouellette	0.32	
FTE Equivalent:	**1.06**	
Total Number:	**3**	

Names of Post Doctorates

NAME	PERCENT_SUPPORTED
Adam Hauser	0.30
FTE Equivalent:	**0.30**
Total Number:	**1**

Names of Faculty Supported

NAME	PERCENT_SUPPORTED	National Academy Member
Leon Balents	0.01	
Susanne Stemmer	0.02	
FTE Equivalent:	**0.03**	
Total Number:	**2**	

Names of Under Graduate students supported

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period:	0.00
The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:......	0.00
The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:......	0.00
Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):......	0.00
Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:......	0.00
The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense	0.00
The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields:......	0.00

Names of Personnel receiving masters degrees

NAME

Total Number:

Names of personnel receiving PHDs

NAME	
Daniel Ouellette	
Ru Chen	
Total Number:	**2**

Names of other research staff

NAME	PERCENT_SUPPORTED
S. James Allen	0.71
Daniel Ouellette	0.16
FTE Equivalent:	**0.87**
Total Number:	**2**

Sub Contractors (DD882)

Inventions (DD882)

Scientific Progress

See attachment.

Technology Transfer

Final Report

Controllable, Hubbard-like Correlated Electron Physics in Oxide Quantum Structures

Proposal Number: 62619-PH-DRP

Agreement Number: W911NF-12-1-0574

Report Date:
November 1, 2014

Principal Investigator:

Susanne Stemmer
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Co-Principal Investigators:

S. James Allen, Leon Balents

Summary

The goal of this project was to determine the conditions under which an excitation gap will form in the electronic states of transition metal oxides due to strong correlations at very high electron densities. We used oxide interfaces as a *tool* to *controllably* probe correlations effects that occur due to short-range interactions at high-electron densities. $SrTiO_3/GdTiO_3$ interfaces served as platform materials system. The project established correlated phenomena that appeared in $SrTiO_3$ quantum wells bound by two $SrTiO_3/GdTiO_3$ interfaces and investigated magnetism in this system.

Summary of Results

Mott Insulating State

$GdTiO_3/SrTiO_3/GdTiO_3$ heterostructures with $SrTiO_3$ thicknesses ranging from ~ 5 nm down to a single SrO layer embedded in $GdTiO_3$ were grown by MBE by the **Stemmer** group. In collaboration with **Balents** and **Allen**, and the **Stemmer** group showed evidence for short-range Coulomb interactions in transport for $SrTiO_3$ quantum wells below ~ 3 SrO layers thickness. An insulating state emerges at two 2 SrO layers [P. Moetakef, et al., Phys. Rev. B **86**, 201102(R) (2012).]. The **Stemmer** group STEM studies of the ultra-narrow quantum wells (1-8 SrO layers) embedded in $GdTiO_3$. We found that layers with 1 and 2 SrO layers, which are insulating, show measurable displacements of Sr sites in the quantum wells. All other quantum wells, containing more than 2 SrO layers, which are metallic, do not show Sr displacements [J. Y. Zhang, et al., Phys. Rev. Lett. **110**, 256401 (2013)]. The observed displacements are in excellent agreement with those predicted by the **Balents** group for this orientation.

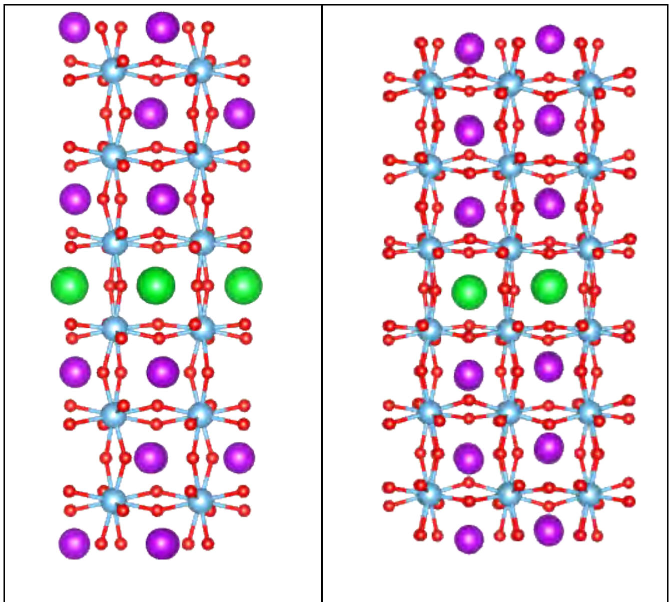

Figure 1: Structure of a single SrO layer embedded in $GdTiO_3$ for [001] growth (left) and [110] growth (right). One observes in the [110] case distinct distortions, e.g. vertical oscillations of the Sr atoms (green sphere), not present for the [001] case.

The **Balents** group carried out theoretical research into emergent order in ultra-thin confined two dimensional oxide structures. The group discovered a dimer Mott insulator (DMI) phase of a single SrO layer in $GdTiO_3$ [R. Chen *et al*, Phys. Rev. B **87**, 161119 (2013)]. In that paper we reported results for the simplest situation, of the orthorhombic material (here $GdTiO_3$) growing along its high symmetry [001] axis. This results in a

situation where the most distorted bonds of the heterostructure are in the growth plane, leading to strong inter-layer exchange that stabilizes dimer formation and hence the DMI.

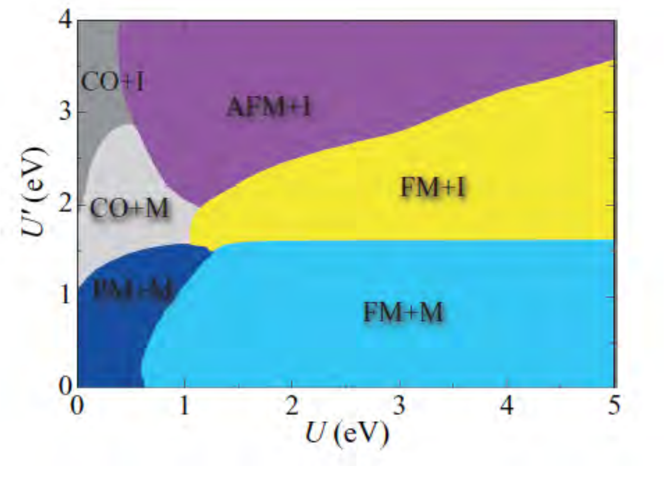

Figure 2: Hartree-Fock phase diagram the DMI. PM+M = paramagnetic metal; CO+M = weakly charge ordered metal; CO+I = charge ordered insulator; FM+M = ferromagnetic metal; FM+I = ferromagnetic insulator; AFM+I = antiferromagnetic insulator [Phys. Rev. B **87**, 161119 (2013)].

For $GdTiO_3$ growing along the [110] axis, which corresponds to the situation studied in the experiment by **Stemmer**, the **Balents** group found that the distortion patterns in the single SrO layer system is quite different in this case, and dimer formation does not appear to be favored. For realistic U values, charge ordering appears to be favorable. This was tentatively identified the charge order as a type of "polaron lattice", and attribute this to a reduced cost of the polaronic lattice deformation around the non-ideal distorted state. The importance of polaron formation was also a result in measurements by the **Allen** group, who determined the in-plane conductivity over a broad frequency range, from DC to optical frequencies, in $SrTiO_3$, quantum wells in the $GdTiO_3$. The **Allen** group found that unlike metallic $SrTiO_3$ quantum wells in $GdTiO_3$, the single SrO delta-doped layer exhibits thermally activated DC and optical conductivity that agree in a quantitative manner with predictions of small polaron transport but with an extremely high two-dimensional density of polarons, 7×10^{14} cm^{-2}. These transport experiments show that the electron or holes in the ground state of this system are ''self-trapped'' as small polarons. [D. G. Ouellette, et al., Sci. Rep. **3**, 3284 (2013)].

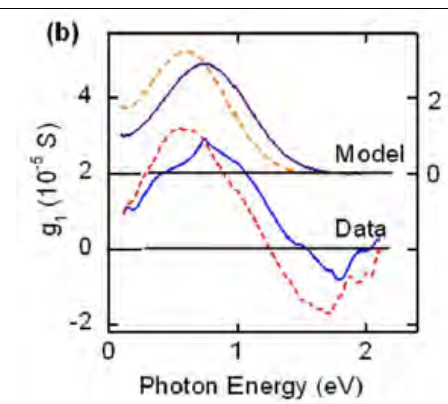

Figure 3: Two-dimensional optical conductivity of the a single SrO layer in $GdTiO_3$ after normalization together with the small polaron model, displaced upward for clarity [Sci. Rep. **3**, 3284 (2013)].

Magnetism

The **Balents** group carried out a study of magnetism in t_{2g}-orbital based electron gases. This work [G. Chen and Leon Balents, Phys. Rev. Lett. **110**, 206401 (2013)], showed that in principle itinerant t_{2g} ferromagnetism is possible in an *intermediate* density range of such systems, but can only support a weak moment and a relatively low critical temperature. Raising the critical temperature would require localization of a large fraction of the electrons. Polaron lattice formation (predicted in theory and shown in the experiment, see above) may indicate that such a path can be possible. We stress that even if polaron localization were achieved, many additional conditions must be met to translate that into substantial magnetic moments.

Stemmer's group investigated the magnetism in $GdTiO_3$/$SrTiO_3$/$GdTiO_3$ heterostructures with $SrTiO_3$ thicknesses ranging from ~ 5 nm down to a single SrO layer embedded in $GdTiO_3$. They showed that the longitudinal and transverse magnetoresistance in the structures with $GdTiO_3$ are consistent with AMR, and thus indicative of induced ferromagnetism in the $SrTiO_3$, rather than a nonequilibrium proximity effect [C. A. Jackson, et al. Phys. Rev. B **88**, 180403(R) (2013)]. The ferromagnetism is a result of exchange coupling, as it does not appear in quantum wells bound by $SmTiO_3$. The ferromagnetic properties of the quantum well are clearly distinct from those of the $GdTiO_3$.

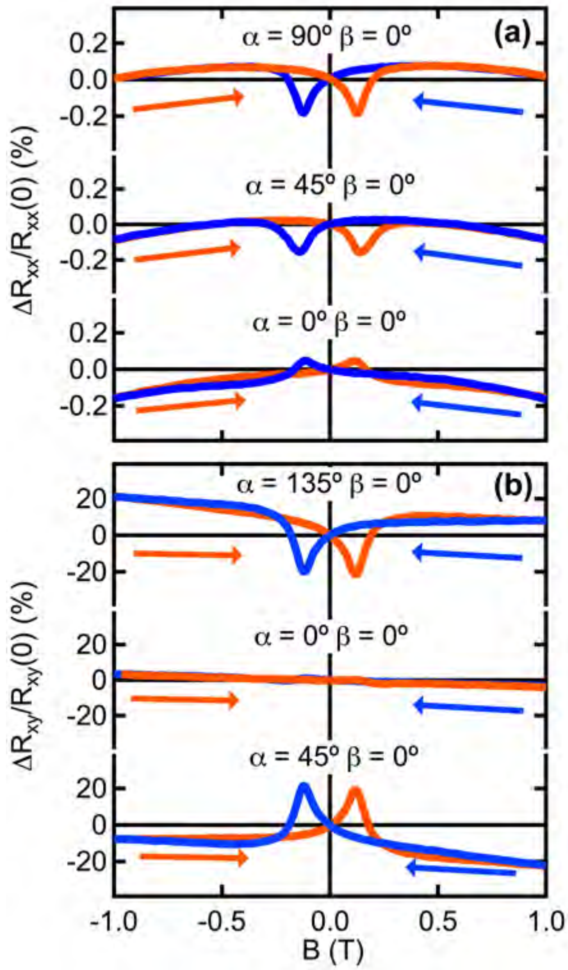

Figure 4: Anisotropic magnetoresistance and hysteresis in ultrathin $SrTiO_3$ quantum wells in $GdTiO_3$. (a) Relative changes in the longitudinal magnetoresistance as a function of in-plane angle α, at $\beta = 0°$. (b) Relative changes in the transverse magnetoresistance as a function of in-plane angle α, at $\beta = 0°$. All measurements are at 2 K [Phys. Rev. B **88**, 180403(R) (2013)].